

10/923,271

<http://www.cas.org/legal/infopolicy.html>

=> file casreact
COST IN U.S. DOLLARS

SINCE FILE	TOTAL
ENTRY	SESSION
0.48	0.69

FULL ESTIMATED COST

FILE 'CASREACT' ENTERED AT 14:13:04 ON 16 JUN 2008
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FILE CONTENT:1840 - 14 Jun 2008 VOL 148 ISS 25

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*****
*
*      CASREACT now has more than 13.8 million reactions      *
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Some CASREACT records are derived from the ZIC/VINITI database (1974-1999) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

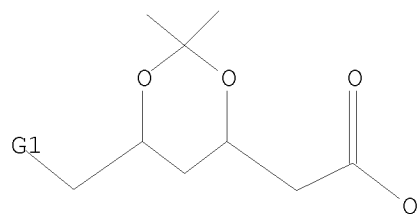
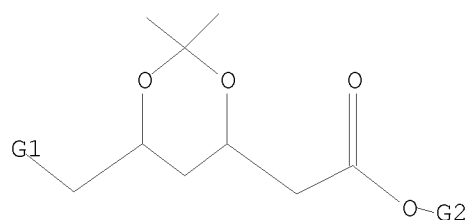
This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\164.str

L1 STRUCTURE UPLOADED

=> d
L1 HAS NO ANSWERS
L1 STR

10/923,271



G1 C, CN, OH

G2 H, Cs, Fr, K, Li, Na, Rb

Structure attributes must be viewed using STN Express query preparation.

=> s l1 full

FULL SEARCH INITIATED 14:13:54 FILE 'CASREACT'

SCREENING COMPLETE - 12038 REACTIONS TO VERIFY FROM 461 DOCUMENTS

100.0% DONE 12038 VERIFIED 133 HIT RXNS

23 DOCS

SEARCH TIME: 00.00.02

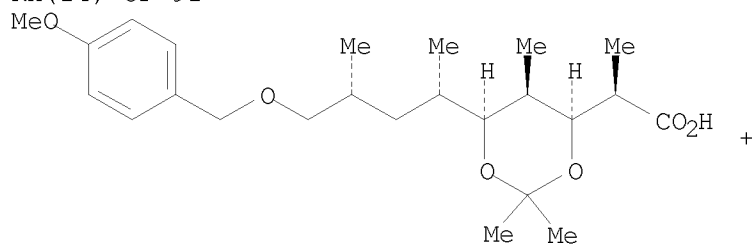
L2 23 SEA SSS FUL L1 (133 REACTIONS)

=> d 1-23

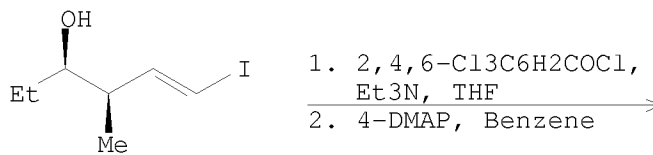
L2 ANSWER 1 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

10/923,271

RX(14) OF 91

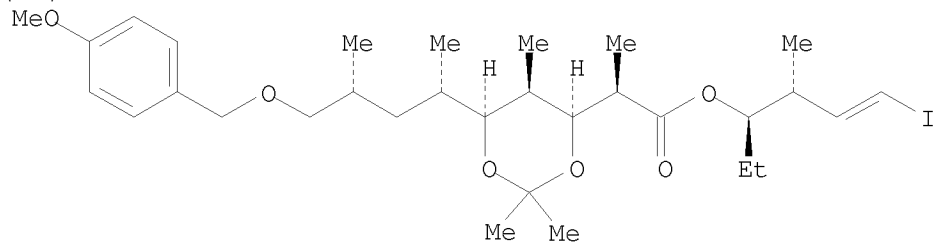


(step 1)



(step 2)

RX(14) OF 91



90%

REF: Journal of Organic Chemistry, 70(18), 7267-7272; 2005

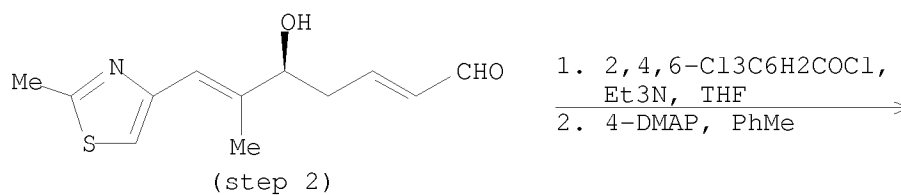
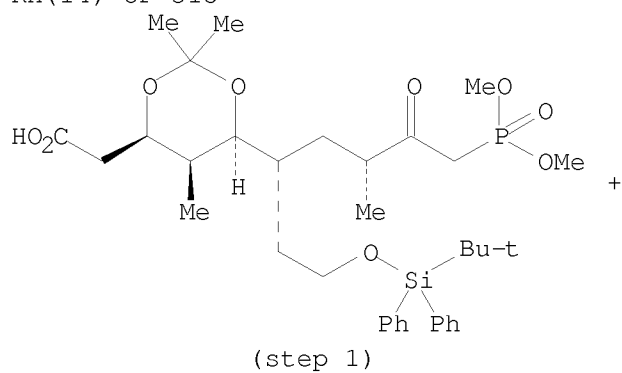
CON: STAGE(1) 2 hours, room temperature

STAGE(2) 24 hours, room temperature

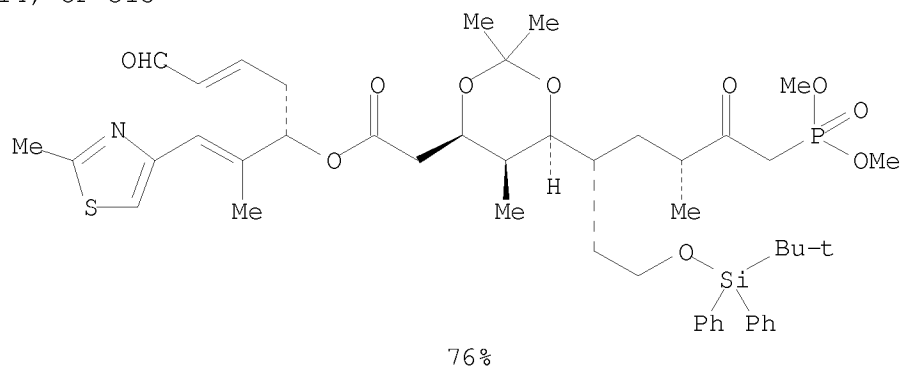
L2 ANSWER 2 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

10/923,271

RX(14) OF 315



RX(14) OF 315

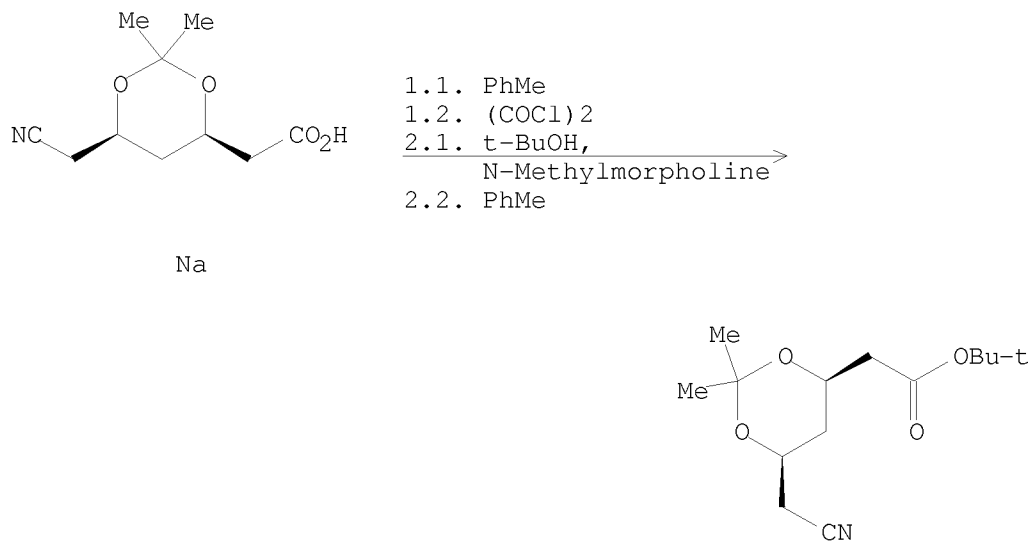


REF: Heterocycles, 64,, 333-345; 2004
CON: STAGE(1) 1 hour, room temperature
STAGE(2) 23 hours, room temperature

L2 ANSWER 3 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(11) OF 18 - 2 STEPS



REF: PCT Int. Appl., 2004096788, 11 Nov 2004

NOTE: 1) first stage Dean Stark app.

CON: STEP(1.1) room temperature

STEP(1.2) 2.5 hours, room temperature; 4 hours, room temperature

STEP(2.1) room temperature

STEP(2.2) 30 minutes, room temperature; 12 hours, room temperature

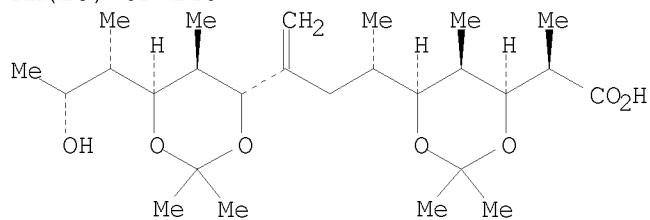
L2 ANSWER 4 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(38) OF 521 - REACTION DIAGRAM NOT AVAILABLE

L2 ANSWER 5 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

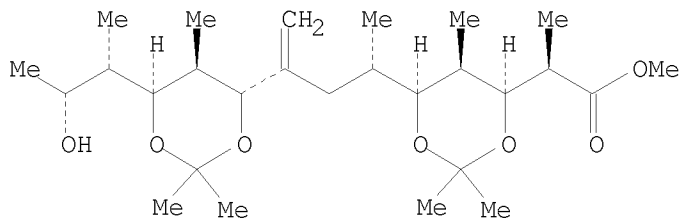
10/923,271

RX(15) OF 140



(step 1)

1. $\text{Me}_3\text{SiCH:N}_2$,
Benzene, MeOH,
Hexane
2. AcOH, Water



100%

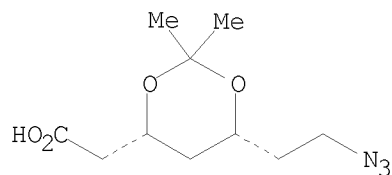
REF: Tetrahedron, 60(21), 4693-4704; 2004

CON: STAGE(1) 45 minutes, room temperature

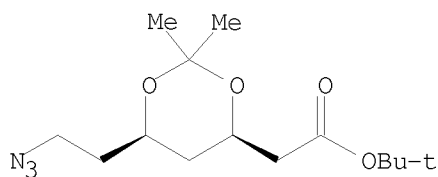
STAGE(2) room temperature

L2 ANSWER 6 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(8) OF 43



(Boc) 2O, 4-DMAP



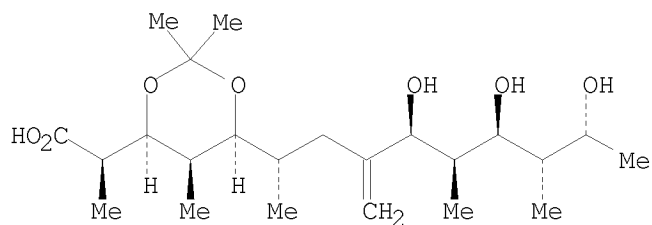
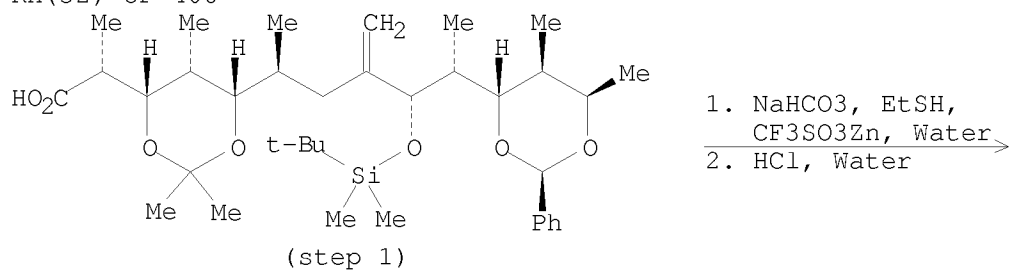
86%

REF: Tetrahedron Letters, 45(11), 2439-2441; 2004

L2 ANSWER 7 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

10/923,271

RX(32) OF 408

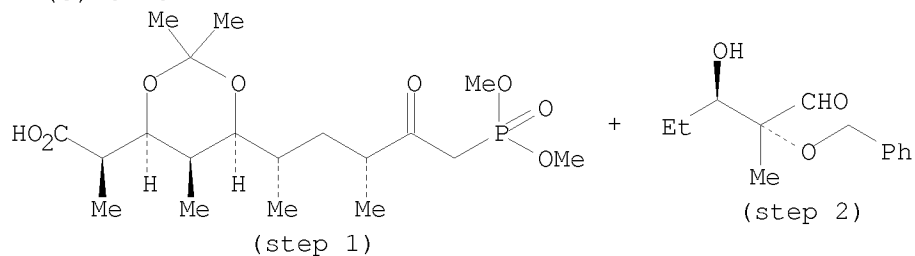


REF: Journal of the American Chemical Society, 124(43), 12806-12815; 2002

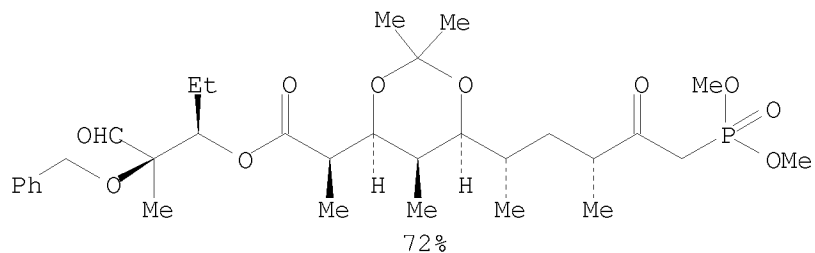
CON: STAGE(1) 2 hours, 0 deg C; 13 hours, room temperature
STAGE(2) pH 4

L2 ANSWER 8 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(5) OF 62



1. 4-DMAP, Et₃N, PhMe



REF: Heterocycles, 46,, 105-110; 1997

NOTE: key step

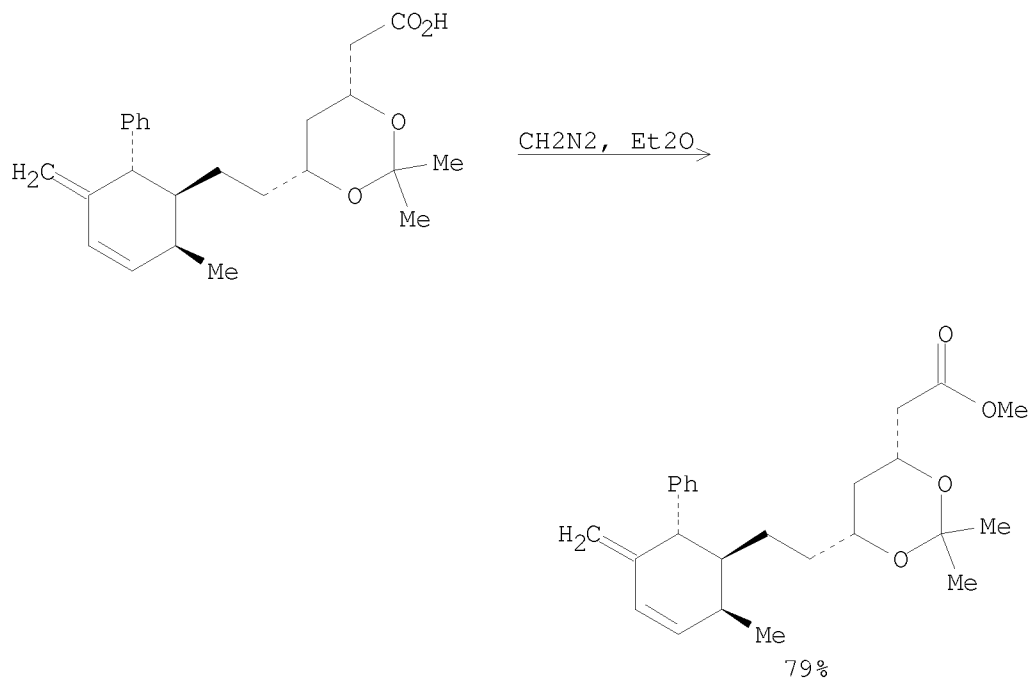
Toh

16/06/2008

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L2 ANSWER 9 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(10) OF 66

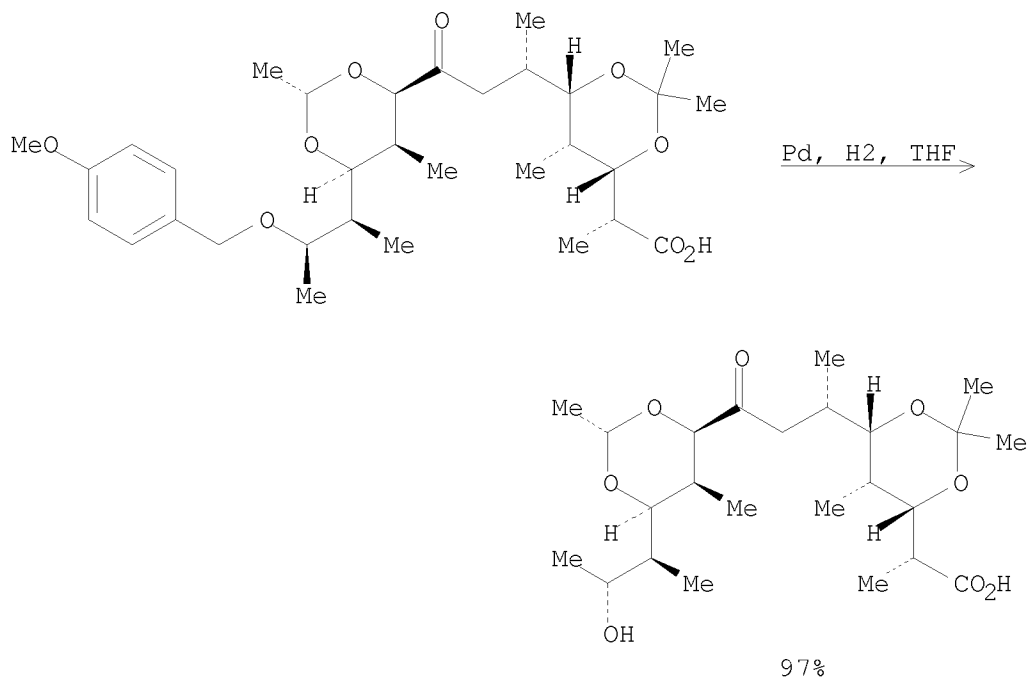


REF: Journal of Organic Chemistry, 60(17), 5532-6; 1995

L2 ANSWER 10 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(39) OF 654

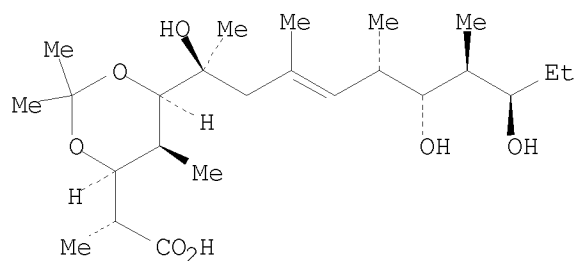


REF: Journal of the American Chemical Society, 116(25), 11287-314;
1994

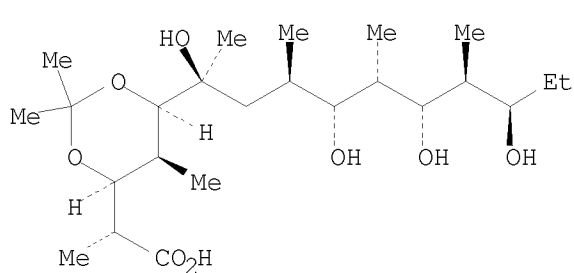
L2 ANSWER 11 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(29) OF 229 - 2 STEPS

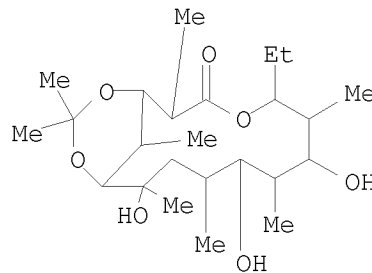


1.1. Et₃N,
2,4,6-Cl₃C₆H₂COCl,
THF
1.2. 4-DMAP, PhMe
2.1. BH₃-Me₂S, THF
2.2. H₂O₂, NaOH,
Water



13%

+



stereoisomers

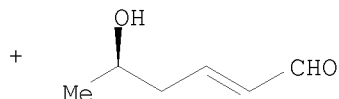
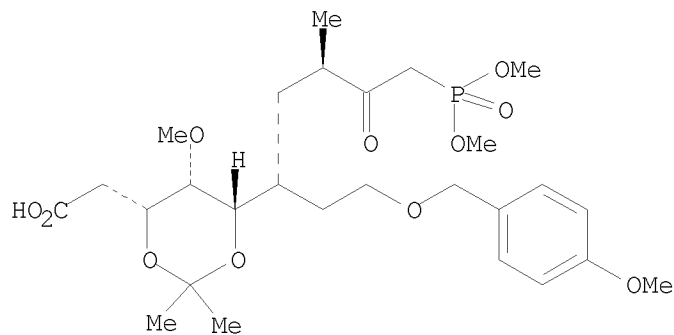
72%

REF: Journal of the American Chemical Society, 113(3), 910-23; 1991

NOTE: 1) 2nd step thermal

L2 ANSWER 12 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(13) OF 306



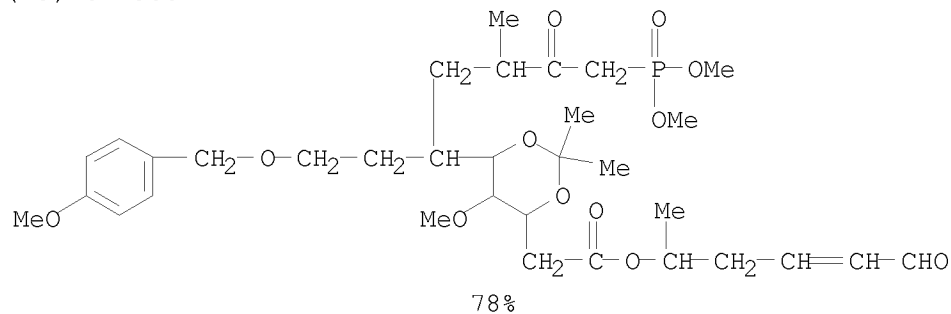
4-DMAP, R:84033-23-8,
PhMe

TOh

16/06/2008

10/923,271

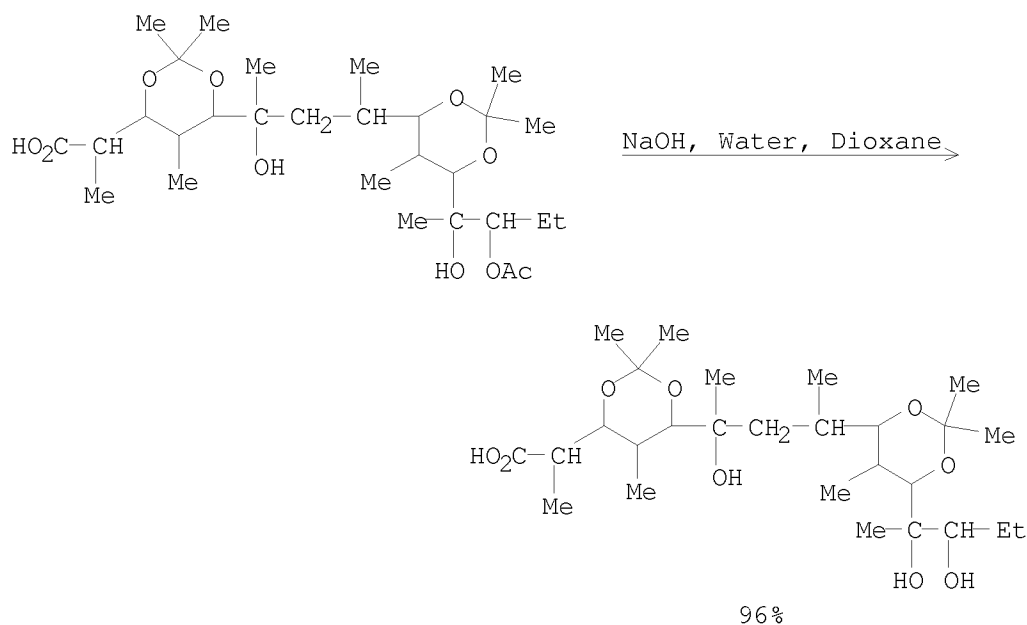
RX(13) OF 306



REF: Heterocycles, 31(1), 5-8; 1990

L2 ANSWER 13 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(65) OF 715

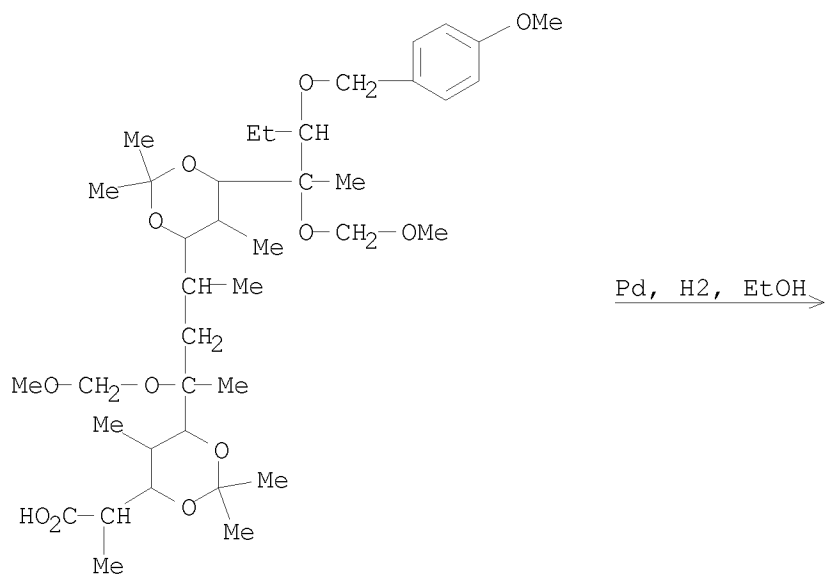


REF: Bulletin of the Chemical Society of Japan, 62(8), 2618-35; 1989

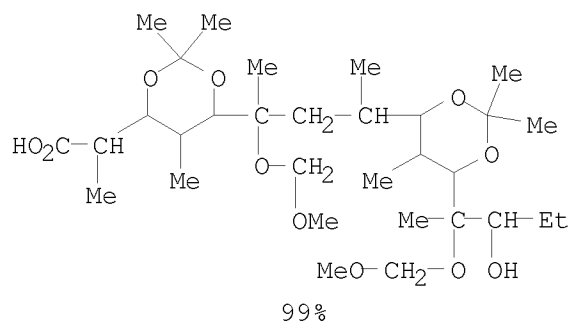
L2 ANSWER 14 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(18) OF 319



RX(18) OF 319

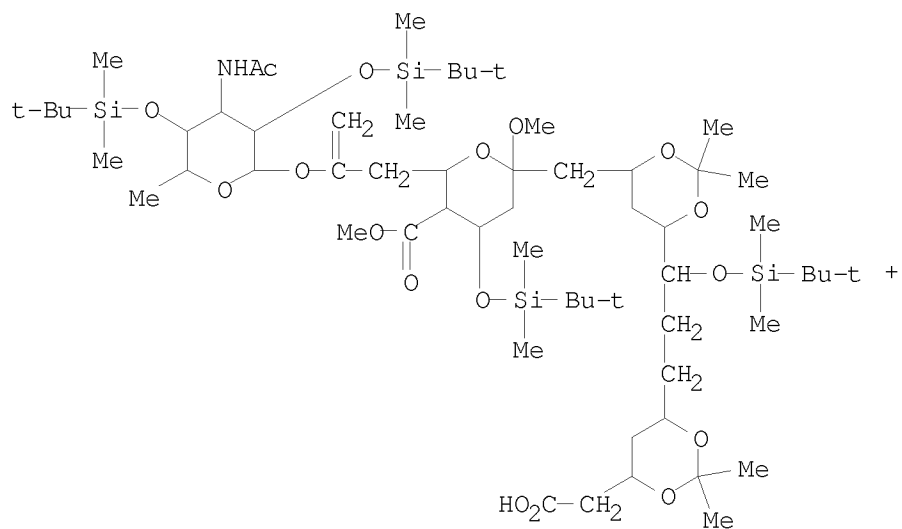


REF: Chemical & Pharmaceutical Bulletin, 37(5), 1167-72; 1989

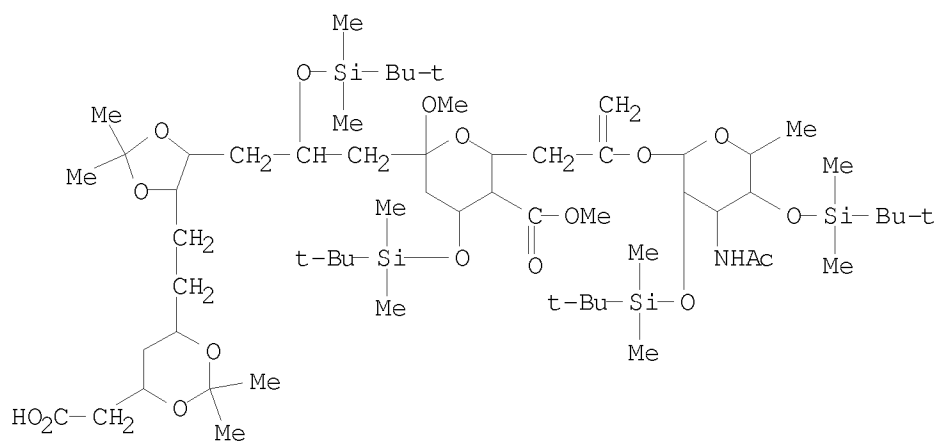
L2 ANSWER 15 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(10) OF 179



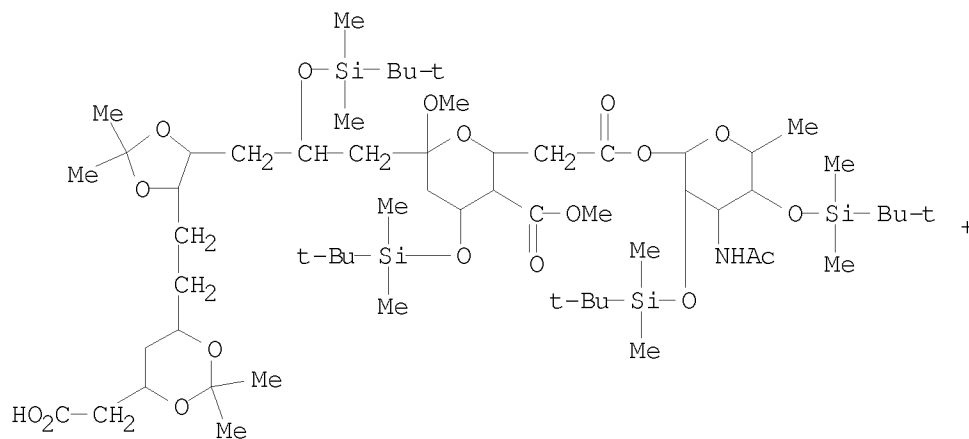
RX(10) OF 179



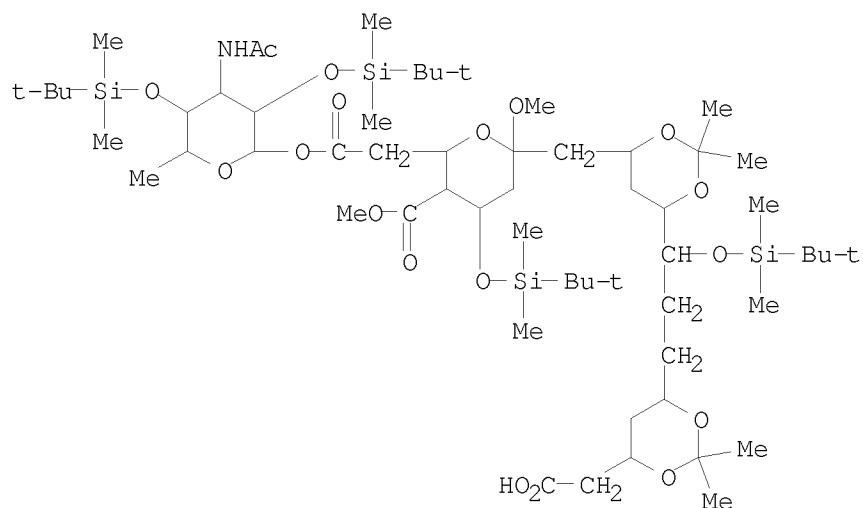
Ozone, MeOH, CH₂Cl₂ →

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RX(10) OF 179



RX(10) OF 179

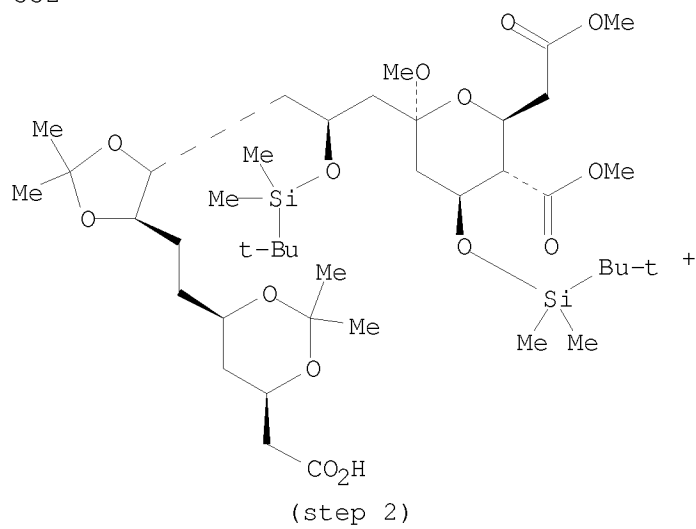


REF: Journal of the American Chemical Society, 110(14), 4660-72; 1988

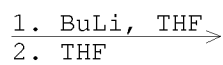
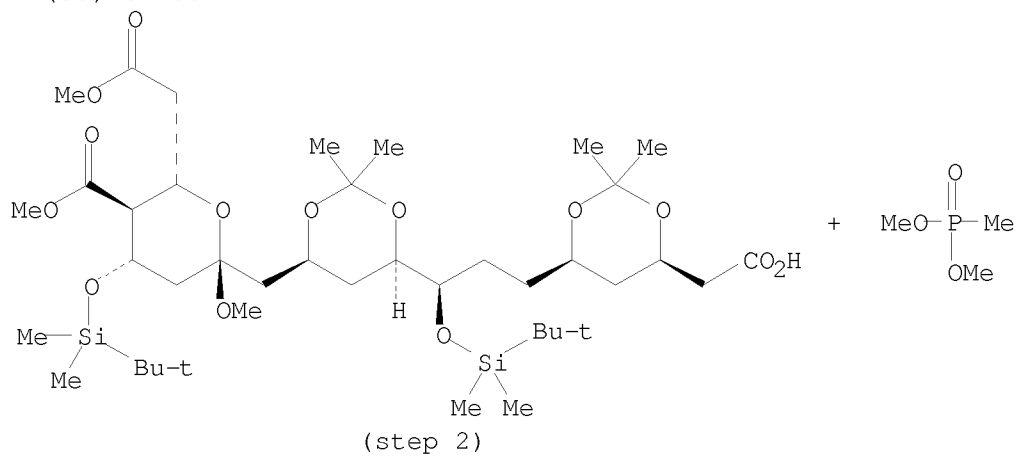
L2 ANSWER 16 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(35) OF 552

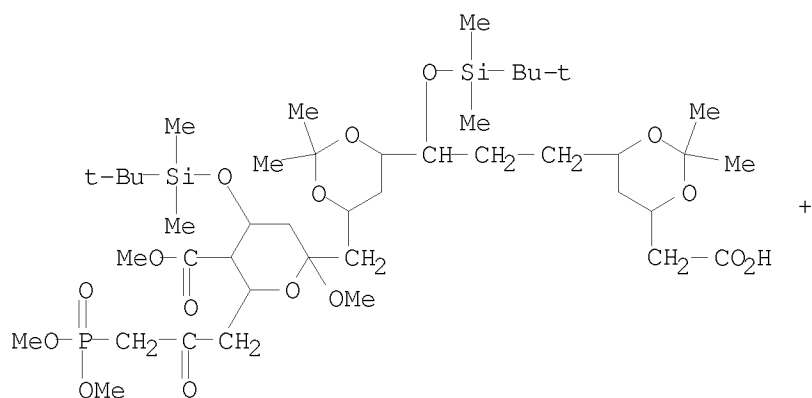


RX(35) OF 552

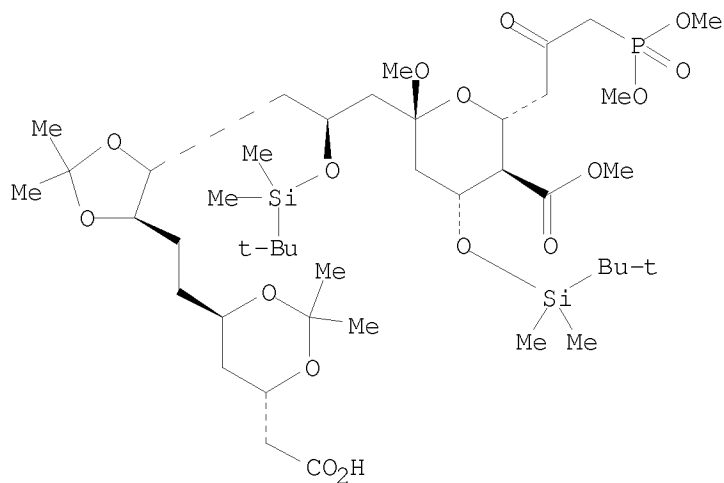


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RX(35) OF 552



RX(35) OF 552



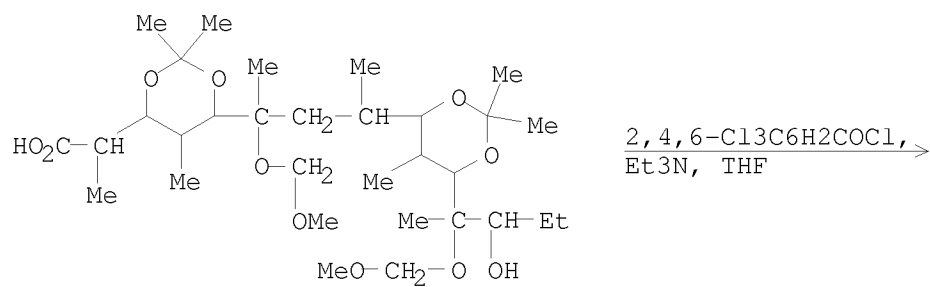
REF: Journal of the American Chemical Society, 110(14), 4685-96;
1988

NOTE: 62% overall

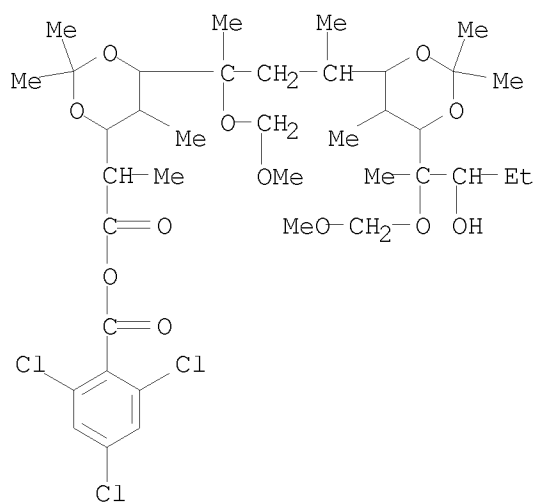
L2 ANSWER 17 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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RX(32) OF 451



RX(32) OF 451



REF: Tetrahedron Letters, 28(39), 4569-72; 1987

L2 ANSWER 18 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(47) OF 265 - REACTION DIAGRAM NOT AVAILABLE

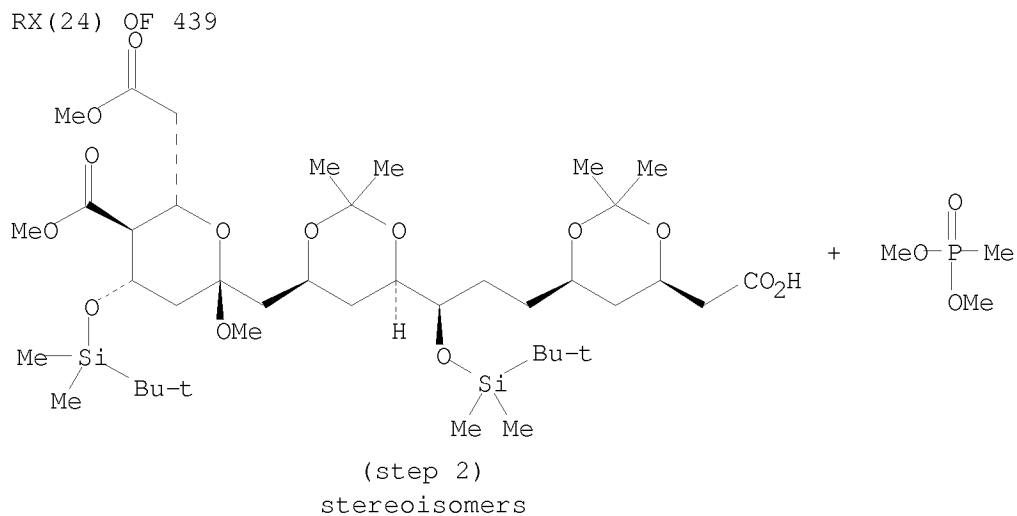
L2 ANSWER 19 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(17) OF 258 - REACTION DIAGRAM NOT AVAILABLE

L2 ANSWER 20 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

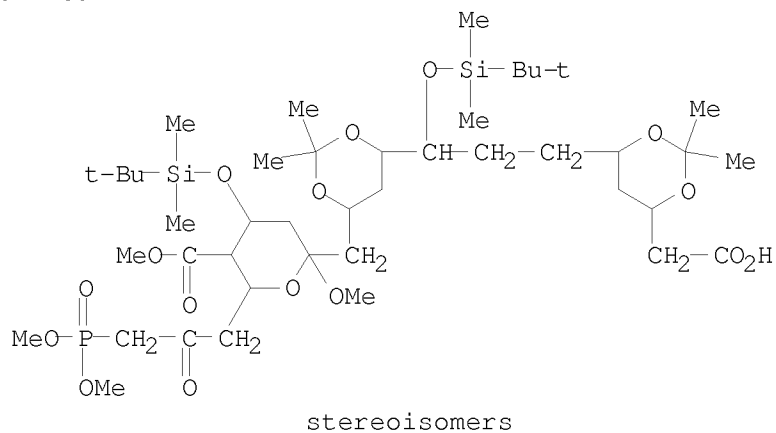
10/923,271

RX(24) OF 439



1. BuLi, THF →

RX(24) OF 439

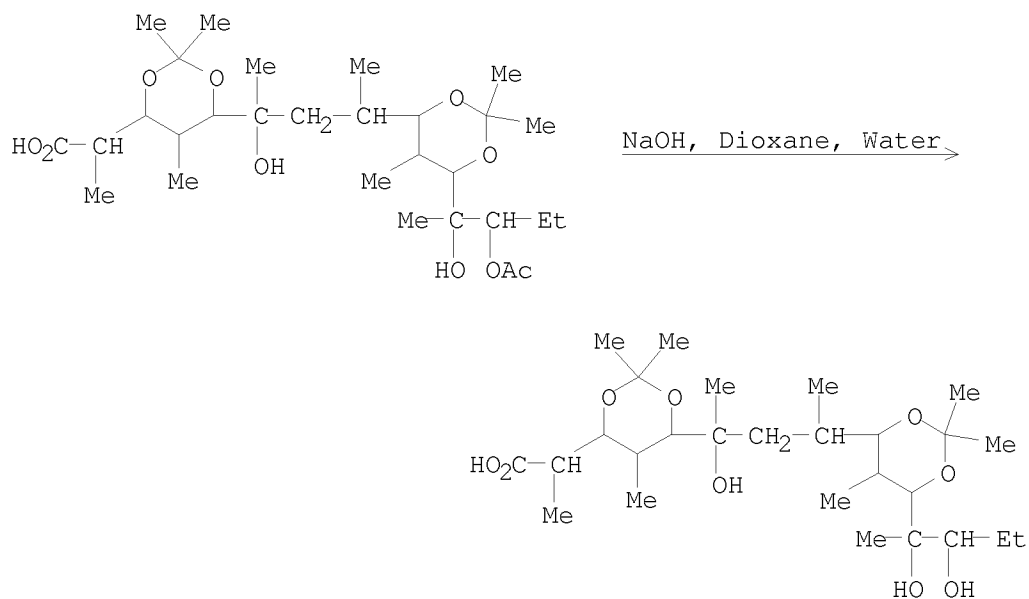


REF: Journal of the American Chemical Society, 109(7), 2208-10; 1987
NOTE: 62% OVERALL

L2 ANSWER 21 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

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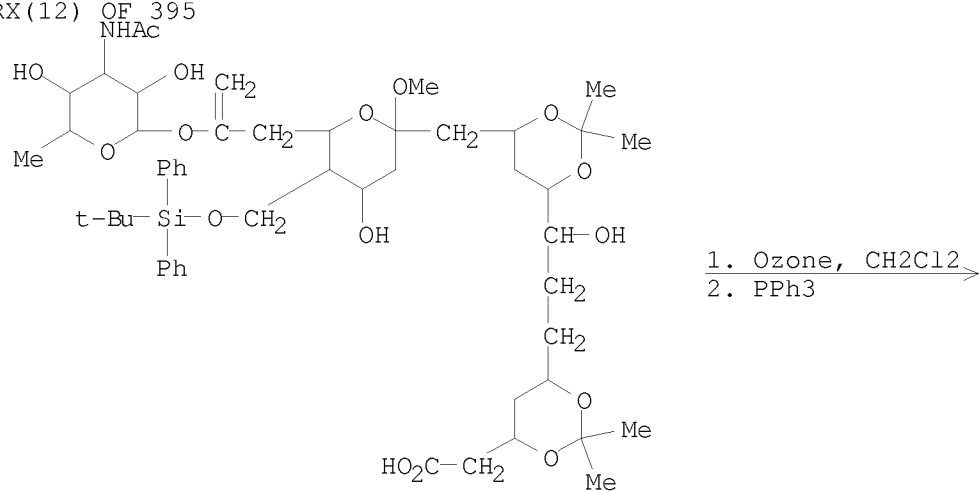
RX(18) OF 316



REF: Tetrahedron Letters, 27(16), 1815-18; 1986

L2 ANSWER 22 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

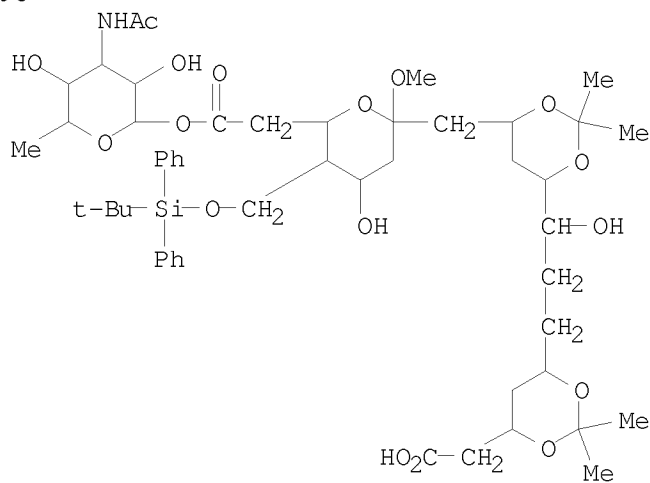
RX(12) OF 395



(step 1)
stereoisomers

10/923,271

RX(12) OF 395

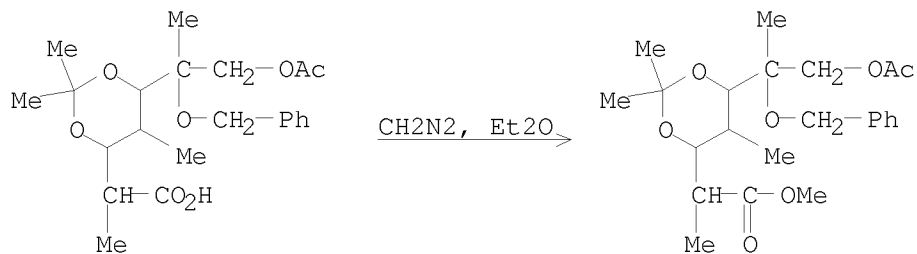


stereoisomers

REF: Journal of the Chemical Society, Chemical Communications, (5), 413-16; 1986

L2 ANSWER 23 OF 23 CASREACT COPYRIGHT 2008 ACS on STN

RX(36) OF 459



REF: Journal of Organic Chemistry, 50(12), 2095-105; 1985